

Optimal packing of spheres in \mathbb{R}^d and extremal effective conductivity

Vladimir Mityushev
Pedagogical University,
ul. Podchorazych 2, Krakow 30-084, Poland

Abstract

Optimal packing of spheres in \mathbb{R}^d is studied by optimization of the energy E (effective conductivity) of composites with ideally conducting spherical inclusions. It is demonstrated that the minimum of E over locations of spheres is attained at the optimal packing. The energy is estimated in the framework of structural approximations. This method yields upper bounds and sometimes exact values for the maximal concentrations of spheres in \mathbb{R}^d . A constructive algorithm for the optimal locations of spheres associated to the classes of the Delaunay graphs is constructed.

Keyword: Optimal packing of spheres; discrete energy; effective conductivity, Voronoi tessellation; Delaunay graph

MSC: 52C17, 05B40, 74Q15

1 Introduction

Packing problems refers to geometrical optimization problems. Various methods from different topics of mathematics were applied to these problems. Extended reviews can be found in the books [3] [4], [5], [7], [11]. One of the most popular problem is the optimal packing of spheres in \mathbb{R}^d [5]. Its complete solution for 2D is given in [11] and for 3D in [7].

It was noted in [9] that solution to the physical problem of the optimal effective conductivity in 2D implies solution to the geometrical problem of the packing disks. The physical problem can be stated as follows. Given ideal conductors (having infinite conductivity coefficient) of the shape $D_i \subset \mathbb{R}^d$ ($i = 1, 2, \dots$). To locate D_i ($i = 1, 2, \dots$) in the host medium of a finite conductivity in such a way that the homogenized medium is macroscopically

isotropic and its effective conductivity attains the minimal value. Rigorous mathematical statements of the physical problem with fixed geometry can be found in [1] and in other works devoted to homogenization.

Recent results in structural approximations [2], [8] shown that densely packed composites can be investigated by the functional associated to the discrete energy. It has the following structure

$$\min_{t_1, t_2, \dots} \sum_{k, j} g_{kj}^{(0)} |t_k - t_j|^2, \quad (1.1)$$

where the minimum is taken over the values t_j prescribed to the inclusion D_j . The value $g_{kj}^{(0)}$ expresses the main term of the interparticle flux between the neighbor inclusions D_j and D_k when the distance δ_{jk} between them tends to zero. Usually, $g_{kj}^{(0)}$ has a simple form. In the case of linear conductivity, $g_{kj}^{(0)}$ not always has a singularity as $\delta_{jk} \rightarrow 0$ (see 3D examples in [8]). For instance, the flux between two spheres in \mathbb{R}^d for $d > 3$ is always regular for linear conductivity. Fortunately, $g_{kj}^{(0)}$ is always singular for non-linear conductivity governed by the p -Laplacian for $p > \frac{d+1}{2}$. This fact enables us to consider the minimum (1.1) not only in t_j but also in the locations of the spherical inclusions D_j .

This paper is devoted to study the minimum (1.1) and its application to the sphere packing problem. Sec.2 shortly presents the structural approximation theory following [6], [2], [8] in \mathbb{R}^d for $d = 2, 3$. Sec.3 is devoted to extension of the theory to the general space \mathbb{R}^d and construction of the corresponding discrete energy. Estimations of energy are performed in Sec.4. Sec.5 contains concluding remarks and discussion.

2 Structural approximation in \mathbb{R}^d

Let $\boldsymbol{\nu}_j$ ($1, 2, \dots, d$) be the fundamental translation vectors in the space \mathbb{R}^d ($d \geq 2$) which form a lattice $\mathcal{Q} = \{\sum_{j=1}^d m_j \boldsymbol{\nu}_j : m_j \in \mathbb{Z}\}$. The fundamental parallelotope Q_0 is defined by its 2^d vertices $\frac{1}{2} \sum_{j=1}^d (\pm \boldsymbol{\nu}_j)$. Two points $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$ are identified if their difference $\mathbf{a} - \mathbf{b} = \sum_{j=1}^d m_j \boldsymbol{\nu}_j$ belongs to the lattice \mathcal{Q} . Hence, such a topology is introduced on Q_0 that the opposite faces are glued. In the case \mathbb{R}^2 , the fundamental parallelogram Q_0 can be considered as the classical flat torus. We will call the introduced topology on Q_0 in \mathbb{R}^d also by toroidal. The distance $\|\mathbf{a} - \mathbf{b}\|$ between two points $\mathbf{a}, \mathbf{b} \in Q_0$ is introduced as

$$\|\mathbf{a} - \mathbf{b}\| := \min_{m_1, \dots, m_d \in \mathbb{Z}} \left\| \mathbf{a} - \mathbf{b} + \sum_{j=1}^d m_j \boldsymbol{\nu}_j \right\|, \quad (2.1)$$

where the modulus means the Euclidean distance between the points \mathbf{a} and \mathbf{b} in \mathbb{R}^d .

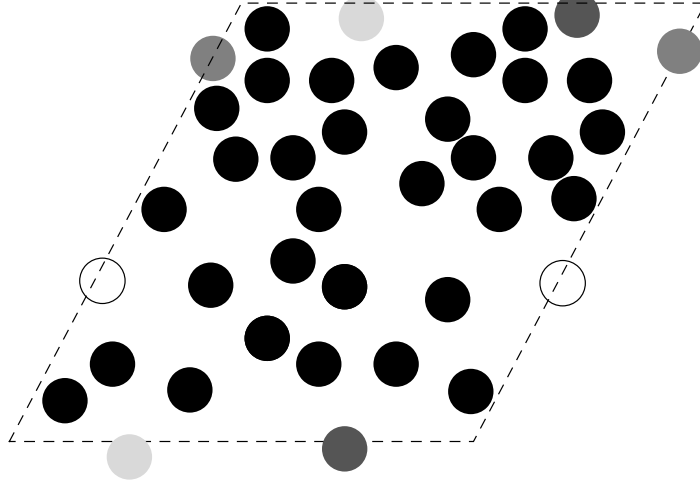


Figure 1: Periodicity cell Q_0 . White and gray balls (disks) are identified in the torus topology.

Consider n non-overlapping balls $D_k = \{\mathbf{x} \in \mathbb{R}^d : |\mathbf{x} - \mathbf{a}_k| < r\}$ of radius r with the centers \mathbf{a}_k in the cell Q_0 (see Fig.1). Let D_0 be the complement of all closure balls $D_k \cup \partial D_k$ to the domain Q_0 . Following [2], [8] and works cited therein we now shortly present the state of art in the non-linear homogenization of periodic composites governed by the p -Laplace equation ($p \geq 2$)

$$\nabla \cdot |\nabla u|^{p-2} \nabla u = 0, \quad \mathbf{x} \in D_0. \quad (2.2)$$

The scalar function $-u(\mathbf{x})$ is called the potential (sometimes the potential is taken as $u(\mathbf{x})$), the vector function $\mathbf{J} = |\nabla u|^{p-2} \nabla u$ is called the flux. The p -Laplace equation (2.2) can be smoothly continued into the perforated domain $D_0 + \sum_{j=1}^d \sum_{m_j \in \mathbb{Z}} m_j \boldsymbol{\nu}_j$. Introduce a unit vector $\boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_d) \in \mathbb{R}^d$. The external potential is determined by the linear function $u_0(\mathbf{x}) = \boldsymbol{\xi} \cdot \mathbf{x}$ up to an arbitrary additive constant. The vector $\boldsymbol{\Omega}_{m_1, \dots, m_d} = \sum_{j=1}^d m_j \xi_j \boldsymbol{\nu}_j$ with $m_j \in \mathbb{Z}$ corresponds to the potential jumps with respect to the lattice \mathcal{Q} , i.e., the potential is quasi-periodic:

$$u \left(\mathbf{x} + \sum_{j=1}^d m_j \boldsymbol{\nu}_j \right) = u(\mathbf{x}) + \boldsymbol{\Omega}_{m_1, \dots, m_d}, \quad \mathbf{x} \in D_0 \quad (\forall m_j \in \mathbb{Z}). \quad (2.3)$$

The flux is periodic:

$$\mathbf{J} \left(\mathbf{x} + \sum_{j=1}^d m_j \boldsymbol{\nu}_j \right) = \mathbf{J}(\mathbf{x}), \quad \mathbf{x} \in D_0 \ (\forall m_j \in \mathbb{Z}). \quad (2.4)$$

The potential satisfies the boundary conditions

$$u(\mathbf{x}) = t_k, \quad |\mathbf{x} - \mathbf{a}_k| = r \ (k = 1, 2, \dots, n), \quad (2.5)$$

where t_k are undetermined constants. The total normal flux through each sphere vanishes:

$$\int_{\partial D_k} \mathbf{J}(\mathbf{x}) \cdot \mathbf{n} \, ds = 0, \quad k = 1, 2, \dots, n, \quad (2.6)$$

where \mathbf{n} denotes the outward unit normal vector to the sphere ∂D_k .

The problem (2.3)-(2.6) describes the field in the periodic composite when the inclusions D_k are occupied by perfect conductor and the host conductivity is governed by equation (2.2). In electrostatics, $\mathbf{E} = \nabla u$ denotes the electric field, $\mathbf{J} = |\nabla u|^{p-2} \nabla u$ the electric current density. Energy passing through the cell per unit volume (effective conductivity) is calculated by formula (6.1.6) from [2]

$$\lambda = \frac{1}{2|Q_0|} \int_{D_0} \mathbf{J} \cdot \mathbf{E} \, d\mathbf{x} = \frac{1}{2|Q_0|} \int_{D_0} |\nabla u|^p \, d\mathbf{x}, \quad (2.7)$$

where $|Q_0|$ stands for the volume of Q_0 . It is assumed that the centers \mathbf{a}_k ($k = 1, 2, \dots, n$) are distributed in Q_0 in such a way that the corresponding composite is isotropic in macroscale, i.e., the effective conductivity of the composite is expressed by a scalar λ and does not depend on the unit external flux $\boldsymbol{\xi}$.

The energy λ can be found as the minimum of the functional [2]:

$$\lambda = \min_{v \in V} \frac{1}{2|Q_0|} \int_{D_0} |\nabla v|^p \, d\mathbf{x}, \quad (2.8)$$

where the space V consists of the quasi-periodic functions from the Sobolev space $W^{1,p}(Q_0)$:

$$V = \{v \in W^{1,p}(Q_0) : v(\mathbf{x}) = t_k \text{ on } D_k \ (k = 1, 2, \dots, n)\}. \quad (2.9)$$

Here, quasi-periodicity means that the conditions (2.3) and (2.4) are fulfilled for v . Though the definition of the space V depends on the external flux $\boldsymbol{\xi}$, the energy does not depend because of isotropy.

The discrete network is a graph Γ on the cell Q_0 with the vertices at \mathbf{a}_k ($k = 1, 2, \dots, n$) and the edges correspond to the necks between neighbors. Neighbors are defined as balls (disks) that share a common edge of the Voronoi tessellation of Q_0 with respect to their centers in toroidal topology. For each fixed \mathbf{a}_k , introduce the set J_k of indexes for neighbor vertices and their total number $N_k = \#J_k$. The Voronoi tessellation in finite domains and the Delaunay graph Γ are precisely described in [2], [8]. The evident modification to periodic structures can be taken over. We use the term the Delaunay graph following [2], [8] because it slightly differs from the Delaunay triangulation in degenerate cases. For example, consider a square and its four vertices. The traditional Delaunay triangulation has four sides of the square and one of the diagonals. In our approach, the Delaunay graph has only four sides (see Example 4.3 in Sec.4).

The discrete network model is based on the justification that the flux is concentrated in the necks between closely spaced inclusions (see [2] for non-linear equation (2.2) and [2], [8] in the linear case $p = 2$). First, we discuss the linear case when $p = 2$. For two balls D_k and D_j the computation of the relative interparticle flux g_{kj} (transport coefficient in terms of [8] and capacity in [6]) relies on Keller's formulae [6]

$$g_{kj} = g_{kj}^{(0)} + O(\delta_{kj}^0), \quad \delta \rightarrow 0, \quad (2.10)$$

where in 3D

$$g_{kj}^{(0)} = -\pi r \ln \delta_{kj} \quad (2.11)$$

and in 2D

$$g_{kj}^{(0)} = \pi \sqrt{\frac{r}{\delta_{kj}}}. \quad (2.12)$$

Here, δ_{kj} denotes the gap between the balls D_k and D_j :

$$\delta_{kj} = \|\mathbf{a}_k - \mathbf{a}_j\| - 2r. \quad (2.13)$$

To each edge of the graph Γ the flux (2.11) or (2.12) is assigned.

In the non-linear case for $p > 2$, we have the following formulae due to [2] in 3D

$$g_{kj}^{(0)} = \frac{\pi}{(p-2)r^{p-3}} \left(\frac{r}{\delta_{kj}} \right)^{p-2} \quad (2.14)$$

and in 2D

$$g_{kj}^{(0)} = \frac{(2p-5)!!}{(2p-4)!!} \frac{\pi^{\frac{3}{2}}}{r^{p-2}} \left(\frac{r}{\delta_{kj}} \right)^{p-\frac{3}{2}}. \quad (2.15)$$

It is worth noting that $g_{kj}^{(0)}$ depends only on geometry of the problem, i.e., on r and on the gap δ_{kj} given by (2.13).

Remark 2.1. The explicit coefficient $\frac{(2p-5)!!}{(2p-4)!!}$ is introduced in (2.15) instead of the coefficient of the Taylor series for $(1-x)^{-\frac{1}{2}}$ in [2]. Formulae (2.14) and (2.15) are taken from [2] with slight corrections (see equations (3.15), (3.17) and a remark below them).

Let for shortness, $\mathbf{t} = (t_1, t_2, \dots, t_n) \in \mathbb{R}^n$ and $\mathbf{a} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n) \in \mathbb{R}^n \times \mathbb{R}^d$. Introduce the double sum

$$\sum'_{k,j} = \sum_{k=1}^n \sum_{j \in J_k}. \quad (2.16)$$

In order to formulate the main asymptotic result of [2] introduce the maximal length of edges $\delta = \max_k \max_{j \in J_k} \delta_{jk}$ of the graph Γ . Following [2], [8] we consider the class \mathcal{D} of macroscopically isotropic composites with densely packed inclusions. The term "densely packed inclusions" means that any such a location of balls has a percolation chain for $\delta = 0$. More precisely, consider a set of non-overlapping balls in Q_0 with $\delta \geq 0$ endowed with the toroidal topology. Change of δ means that the centers of balls are fixed but their radii change and remain equal. Let for $\delta = 0$ there exists a chain of touching balls connecting the opposite faces of the parallelotope Q_0 . Such a chain is called a percolation chain¹. Macroscopic isotropy implies that each pair of the opposite faces of Q_0 posses a percolation chain for $\delta = 0$ (see Fig.2). Any macroscopically isotropic location not belonging to the class \mathcal{D}

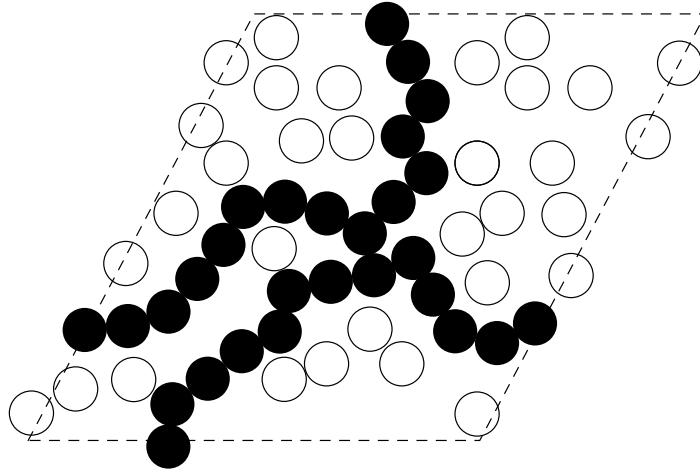


Figure 2: Percolation chains marked by black.

¹In the percolation theory, a percolation chain of balls is usually defined as a chain of overlapping open balls.

of densely packed inclusions can be replaced by an element of \mathcal{D} having higher concentration. It is possible to do it by parallel translations of non-touching groups of balls to make them touched.

Introduce the main term of the discrete energy [2]

$$\sigma = \min_{\mathbf{t}} \frac{1}{2|Q_0|} \sum'_{k,j} g_{kj}^{(0)} |t_k - t_j|^p, \quad (2.17)$$

where $g_{kj}^{(0)}$ is given by (2.14) or by (2.15).

Theorem 2.2 ([2]). *The continuous energy (2.7) and the discrete energy (2.17) for $p \geq 2$ in the spaces \mathbb{R}^d ($d = 2, 3$) tend to $+\infty$ as $\delta \rightarrow +0$. Moreover, λ can be approximated by σ for sufficiently small δ :*

$$\lambda = \sigma + O(\delta^0), \text{ as } \delta \rightarrow 0. \quad (2.18)$$

Th.2.2 justifies the theory of structural approximation [2], [8] based on a mesoscopic discretization when edges and vertices of the graph Γ correspond to inclusions. This theorem was applied in [2], [8], [10] to systematic study of densely packed composites with given locations of inclusions.

3 Discrete network in \mathbb{R}^d

Though the theory of structural approximation [2], [8], [10] was constructed and justified in \mathbb{R}^2 and in \mathbb{R}^3 , its main results hold in the general space \mathbb{R}^d under the condition that the interparticle flux g_{kj} tends to infinity as $\delta_{kj} \rightarrow 0$. It can be established by a formal repetition of the arguments from [2], [8] in \mathbb{R}^d . In the present section, we partially fill this gap and calculate the main term $g_{kj}^{(0)}$ of g_{kj} up to a constant order term $O(\delta_{jk}^0)$.

Following Keller [6] and explanations by Kolpakov [8, p. 18-25] we proceed to estimate the interparticle flux g_{jk} for two balls D_j and D_k with the centers located at the points $(0, 0, \dots, 0, \pm \frac{a}{2})$ of radius $r < \frac{a}{2}$ in \mathbb{R}^d ($d = 2, 3, \dots$). Let the potential $u(\mathbf{x})$ is equal to constants $\pm C$ on the spheres $(x_d \mp \frac{a}{2})^2 + R^2 = r^2$ where $R = \sqrt{x_1^2 + x_2^2 + \dots + x_{d-1}^2}$. Near the gap the spheres can be approximated by the paraboloids [2], [8]

$$x_n = \pm \left(\frac{\delta_{jk}}{2} + \frac{R^2}{2r} \right), \quad (3.1)$$

where $\delta_{jk} = a - 2r$. The potential can be approximated up to $O(\delta_{jk}^0)$ by the function (see (6.4.12) from [2] for 2D and 3D cases)

$$u_0(\mathbf{x}) = \frac{x_d}{H(\mathbf{x}_{d-1})}, \quad (3.2)$$

where $H(\mathbf{x}_{d-1}) = \delta + \frac{R^2}{r}$ is the distance between the paraboloids. Following [2] we can approximate the local gradient by

$$\nabla u_0(\mathbf{x}) = \left(0, \dots, 0, \frac{1}{\delta_{jk} + \frac{R^2}{r}}\right) + O(\delta_{jk}^0) \quad (3.3)$$

and the local flux by

$$|\nabla u_0(\mathbf{x})|^{p-2} \nabla u_0(\mathbf{x}) = \left(0, \dots, 0, \frac{1}{\left(\delta_{jk} + \frac{R^2}{r}\right)^{p-1}}\right) + O(\delta_{jk}^0). \quad (3.4)$$

Then, g_{jk} is approximated up to $O(\delta_{jk}^0)$ by the integral over the $(d-1)$ -dimensional ball B on the hyperplane $x_d = 0$ defined by inequality $R < r$:

$$g_{jk}^{(0)} = \int_B \frac{d\mathbf{x}_{d-1}}{\left(\delta_{jk} + \frac{R^2}{r}\right)^{p-1}}, \quad (3.5)$$

where the differential $d\mathbf{x}_{d-1} = dx_1 dx_2 \cdots dx_{d-1}$.

First, we consider partial cases of (3.5) discussed in the previous works [6], [2], [8]. Let $p = d = 2$. Then, (3.5) becomes

$$g_{jk}^{(0)} = \int_{-r}^r \frac{dR}{\delta + \frac{R^2}{r}} = \pi \sqrt{\frac{r}{\delta_{jk}}}. \quad (3.6)$$

Let $p = 2$ and $d = 3$. Then, (3.5) gives

$$g_{jk}^{(0)} = 2\pi \int_0^r \frac{R dR}{\delta_{jk} + \frac{R^2}{r}} = \pi r \ln \frac{r}{\delta_{jk}}. \quad (3.7)$$

Formulae (3.6)-(3.7) coincide with the corresponding formulae from [6], [2], [8] (see also (2.11)-(2.12)).

We now proceed to investigate the general case. The integral (3.5) in the spherical coordinates $(R, \phi_1, \phi_2, \dots, \phi_{d-2})$ becomes

$$g_{jk}^{(0)} = \int_0^{2\pi} d\phi_{d-2} \int_0^\pi d\phi_{d-3} \cdots \int_0^\pi d\phi_1 \int_0^r \frac{\sin^{d-3} \phi_1 \sin^{d-4} \phi_2 \cdots \sin \phi_{d-3}}{\left(\delta + \frac{R^2}{r}\right)^{p-1}} R^{d-2} dR. \quad (3.8)$$

It can be calculated analogously to the volume of the d -dimensional ball. First, calculate

$$\int_0^{2\pi} d\phi_{d-2} \int_0^\pi d\phi_{d-3} \cdots \int_0^\pi \sin^{d-3} \phi_1 \sin^{d-4} \phi_2 \cdots \sin \phi_{d-3} d\phi_1 = \frac{2\pi^{\frac{d-1}{2}}}{\Gamma\left(\frac{d-1}{2}\right)}, \quad (3.9)$$

where the Γ -function is used. The integral in R is calculated by formula

$$\int_0^r \frac{R^{d-2} dR}{\left(\delta_{jk} + \frac{R^2}{r}\right)^{p-1}} = \frac{r^{d-1} {}_2F_1\left(\frac{d-1}{2}, p-1, \frac{d+1}{2}, -\frac{r}{\delta_{jk}}\right)}{\delta_{jk}^{p-1}(d-1)}, \quad (3.10)$$

where the hypergeometric function ${}_2F_1$ is used. Therefore,

$$g_{jk} = \frac{2\pi^{\frac{d-1}{2}} r^{d-1} {}_2F_1\left(\frac{d-1}{2}, p-1, \frac{d+1}{2}, -\frac{r}{\delta_{jk}}\right)}{\Gamma\left(\frac{d-1}{2}\right) \delta_{jk}^{p-1}(d-1)}. \quad (3.11)$$

Hereafter, we assume that p is a natural number greater than 2 and

$$p > \frac{d+1}{2}. \quad (3.12)$$

The following asymptotic formula takes place for $Z \rightarrow \infty$

$${}_2F_1\left(\frac{d-1}{2}, p-1, \frac{d+1}{2}, -Z\right) = \frac{1}{Z^{\frac{d-1}{2}}} \frac{\Gamma\left(\frac{d+1}{2}\right) \Gamma\left(p - \frac{d+1}{2}\right)}{\Gamma(p-1)} + O\left(\frac{1}{Z^q}\right), \quad (3.13)$$

where $q > \frac{d-1}{2}$. Formula (3.13) is got by use of the package *Mathematica*[®]. Applying (3.13) to (3.11) we obtain the main asymptotic term of g_{jk} as $\delta_{jk} \rightarrow 0$

$$g_{jk}^{(0)} = \frac{1}{\delta_{jk}^{p-\frac{d+1}{2}}} \frac{2(\pi r)^{\frac{d-1}{2}} \Gamma\left(\frac{d+1}{2}\right) \Gamma\left(p - \frac{d+1}{2}\right)}{(d-1) \Gamma\left(\frac{d-1}{2}\right) \Gamma(p-1)}. \quad (3.14)$$

Let d be an odd number. Then, (3.14) becomes

$$g_{jk}^{(0)} = \frac{1}{\delta_{jk}^{p-\frac{d+1}{2}}} \frac{(\pi r)^{\frac{d-1}{2}} (p - \frac{d+3}{2})!}{(p-2)!}. \quad (3.15)$$

Let d be an even number. Using formula

$$\Gamma\left(\frac{m}{2}\right) = \frac{(m-2)!! \sqrt{\pi}}{2^{\frac{m-1}{2}}}, \quad m \in \mathbb{N}, \quad (3.16)$$

we rewrite (3.14) in the form²

²Our formulae (3.14), (3.15) and (3.17) slightly diverge with the corresponding formulae from [2] (see for instance (6.2.13)) by multipliers. It can be related to the error power p taken in [2] (e.g. (6.4.15) from [2] for 2D and 3D cases) instead of the correct $p-1$ from (3.5).

$$g_{jk}^{(0)} = \frac{1}{\delta_{jk}^{p-\frac{d+1}{2}}} \frac{\sqrt{\pi}(\pi r)^{\frac{d-1}{2}}(2p-d-3)!!}{2^{p-\frac{d+1}{2}}(p-2)}. \quad (3.17)$$

Introduce the functional associated with energy

$$E(\mathbf{t}, \mathbf{a}) = \frac{1}{2|Q_0|} \sum'_{k,j} (t_k - t_j)^p f(\|\mathbf{a}_k - \mathbf{a}_j\|) \quad (3.18)$$

and the main term of the discrete energy

$$\sigma = \min_{\mathbf{t}} \frac{1}{2|Q_0|} \sum'_{k,j} (t_k - t_j)^p f(\|\mathbf{a}_k - \mathbf{a}_j\|). \quad (3.19)$$

Here, the main term of the interparticle flux $g_{jk}^{(0)}$ is written through the function $f(x) = c(x - 2r)^{-(p-\frac{d+1}{2})}$ of one variable $x \geq 0$. The constant c depends on r, p, d and can be explicitly written by use of (3.15), (3.17). Th.2.2 can be extended to the general space \mathbb{R}^d as follows.

Theorem 3.1. *Consider the class \mathcal{D} of densely packed balls in \mathbb{R}^d . The continuous energy (2.7) (see also (2.8)) and the discrete energy (3.19) for $p \in \mathbb{N}$ satisfying (3.12) tend to $+\infty$ as $\delta \rightarrow +0$. Moreover, λ can be approximated by σ for sufficiently small δ :*

$$\lambda = \sigma + O(\delta^0), \text{ as } \delta \rightarrow 0. \quad (3.20)$$

Proof of the theorem repeats the proof of Th.2.2 from [2] by its extension to the periodicity cell Q_0 in the space \mathbb{R}^d .

Theorem 3.2. *Consider the class \mathcal{D} of densely packed balls in \mathbb{R}^d . Let $\sigma = \sigma(\mathbf{a})$ attains the global minimum at a location $\mathbf{a}_*(\delta)$ for sufficiently small δ . Then, the optimal packing is attained at $\mathbf{a}_*(0)$.*

Proof. Let $\sigma(\mathbf{a})$ attain the global minimum at $\mathbf{a}_*(\delta)$ for sufficiently small δ and ϕ_* denote the concentration of balls for the location $\mathbf{a}_*(0)$. The function $\sigma(\mathbf{a})$ continuously depends on concentration [2], [8]. Hence, the function $\sigma(\mathbf{a}_*(\delta))$ is continuous in $0 < \delta < \delta_0$ for sufficiently small δ_0 and $\sigma(\mathbf{a}_*(0)) = +\infty$.

Let the optimal packing be attained at another location \mathbf{a}^* for which the concentration $\phi^* > \phi_*$. The location \mathbf{a}^* contains a percolation chain. Take such a radius $r_0 < r$ for which the concentration is reduced to ϕ_* . Then, all the balls in this location \mathbf{a}^* with the radius r_0 are separated from each other, hence the corresponding conductivity $\sigma(\mathbf{a}^*)$ is a finite number. But the minimal conductivity $\sigma(\mathbf{a}_*(\delta))$ tends to infinity as $\delta \rightarrow 0$. This yields a contradiction.

The theorem is proved.

4 Extremal energy

Let all the periodic Delaunay graphs Γ with n vertices are divided onto the equivalence classes of isomorphic graphs. A class of graphs will be denoted by \mathcal{G} . We are looking for the global minimum of the functional (3.18) in \mathbf{t} and \mathbf{a} in the torus topology:

$$\min_{\mathbf{t}, \mathbf{a}} E(\mathbf{t}, \mathbf{a}) = \sum'_{k,j} |t_k - t_j|^p f(\|\mathbf{a}_k - \mathbf{a}_j\|) \quad (4.1)$$

in a fixed class \mathcal{G} .

It is evident that the minimum (4.1) exists since the continuous function $f(x)$ decreases and $0 \leq f(\|\mathbf{a}_k - \mathbf{a}_j\|) \leq +\infty$ for all $\|\mathbf{a}_k - \mathbf{a}_j\| \geq 2r$. The function $f(x)$ as a convex function for $2r \leq x < +\infty$ satisfies Jensen's inequality

$$\sum_{i=1}^M p_i f(x_i) \geq f\left(\sum_{i=1}^M p_i x_i\right), \quad (4.2)$$

where the sum of positive numbers p_i is equal to unity. Equality holds if and only if all x_i are equal. Let the finite sum $\sum'_{k,j}$ in (4.1) is arranged in such a way that $x_i = \|a_k - a_j\|$ and $p_i = \frac{1}{T}(t_k - t_j)^p$, where $T = \sum'_{k,j} (t_k - t_j)^p$.

Application of (4.2) yields

$$\sum'_{k,j} (t_k - t_j)^p f(\|\mathbf{a}_k - \mathbf{a}_j\|) \geq T f\left(\frac{1}{T} \sum'_{k,j} (t_k - t_j)^p \|\mathbf{a}_k - \mathbf{a}_j\|\right). \quad (4.3)$$

Hölder's inequality states that for non-negative a_i and b_i

$$\sum_{i=1}^M a_i b_i \leq \left(\sum_{i=1}^M a_i^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^M b_i^2\right)^{\frac{1}{2}}. \quad (4.4)$$

This implies that

$$\sum'_{k,j} (t_k - t_j)^p \|\mathbf{a}_k - \mathbf{a}_j\| \leq \left[\sum'_{k,j} (t_k - t_j)^{2p}\right]^{\frac{1}{2}} \left[\sum'_{k,j} \|\mathbf{a}_k - \mathbf{a}_j\|^2\right]^{\frac{1}{2}}. \quad (4.5)$$

The function $f(x)$ decreases, hence (4.3) and (4.5) give

$$\sum'_{k,j} (t_k - t_j)^p f(\|a_k - a_j\|) \geq T f\left(\frac{1}{T} \left[\sum'_{k,j} (t_k - t_j)^{2p}\right]^{\frac{1}{2}} \left[\sum'_{k,j} \|a_k - a_j\|^2\right]^{\frac{1}{2}}\right). \quad (4.6)$$

The minimum of the right hand part of (4.6) on $\mathbf{a} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n)$ is achieved independently on t_k for

$$\max_{\mathbf{a}} g(\mathbf{a}) = \sum'_{k,j} \|\mathbf{a}_k - \mathbf{a}_j\|^2. \quad (4.7)$$

Lemma 4.1. *For any fixed n , any local maximizer of $g(\mathbf{a})$ is the global maximizer which fulfils the system of linear algebraic equations*

$$\mathbf{a}_k = \frac{1}{N_k} \sum_{j \in J_k} \mathbf{a}_j + \frac{1}{N_k} \sum_{\ell=1}^d s_{j\ell} \boldsymbol{\nu}_\ell, \quad k = 1, 2, \dots, n, \quad (4.8)$$

where $s_{j\ell}$ can take the values $0, \pm 1$ in accordance with the fixed Voronoi tessellation (the fixed graph Γ). The system (4.8) has always a unique solution $\mathbf{a} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n)$ up to an arbitrary additive constant vector.

Proof. It follows from the definition (2.1) and the properties of the Voronoi tessellation that

$$\|\mathbf{a}_k - \mathbf{a}_j\| = \left\| \mathbf{a}_k - \mathbf{a}_j + \sum_{\ell=1}^d s_{j\ell} \boldsymbol{\nu}_\ell \right\| \quad (4.9)$$

for some $s_{j\ell}$ which can take the values $0, \pm 1$. The extremal points of (4.7) can be found from the system of equations

$$\nabla_k g(\mathbf{a}) = 0, \quad k = 1, 2, \dots, n, \quad (4.10)$$

where $\mathbf{a}_k = (x_1^{(k)}, x_2^{(k)}, \dots, x_d^{(k)})$ and

$$\nabla_k = \left(\frac{\partial}{\partial x_1^{(k)}}, \frac{\partial}{\partial x_2^{(k)}}, \dots, \frac{\partial}{\partial x_d^{(k)}} \right)$$

The parallelotope Q_0 is a compact manifold without boundary, hence all the extremal points of (4.7) satisfy this system. Equations (4.10) can be written in the equivalent form (4.8).

One can see that the sum of all equations (4.8) gives an identity, hence, they are linearly dependent. Moreover, if $\mathbf{a} = (\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n)$ is a solution of (4.8), then $(\mathbf{a}_1 + \mathbf{c}, \mathbf{a}_2 + \mathbf{c}, \dots, \mathbf{a}_n + \mathbf{c})$ is also a solution of (4.8) for any $\mathbf{c} \in \mathbb{R}^d$. Consider the homogeneous system corresponding to (4.8)

$$\mathbf{a}_k = \frac{1}{N_k} \sum_{j \in J_k} \mathbf{a}_j, \quad k = 1, 2, \dots, n, \quad (4.11)$$

where \mathbf{a}_k belong to the cell Q_0 . The system (4.11) can be decoupled by coordinates onto independent systems

$$x_p^{(k)} = \frac{1}{N_k} \sum_{j \in J_k} x_p^{(j)}, \quad k = 1, 2, \dots, n \quad (p = 1, 2, \dots, d). \quad (4.12)$$

Each p th system (4.12) has only constant solutions

$$x_p^{(1)} = x_p^{(2)} = \dots = x_p^{(n)}. \quad (4.13)$$

This follows from the consideration of the quadratic form

$$X_p = \frac{1}{2} \sum'_{k,j} (x_p^{(k)} - x_p^{(j)})^2. \quad (4.14)$$

It is symmetric and positive semi-definite. Therefore, the quadratic form (4.12) has a global minimum attained at a linear set of \mathbb{R}^n . All the local minima of (4.12) coincide with the global minimum. One can see that the quadratic form attains the global minimum at the set (4.13). Therefore, all solutions of (4.12), hence, of (4.11) are only constants. Then, the system (4.8) has only one condition of solvability for the right hand part which is fulfilled. Therefore, the system (4.8) always has a unique solution up to an arbitrary additive constant.

The lemma is proved.

We now proceed to summarize the obtained results concerning the geometrical optimal packing problem of equal spheres stated for periodic packing in \mathbb{R}^d . We consider the periodicity cell Q_0 represented by a parallelotope with glued opposite faces which contains an arbitrary number n of spheres. The centers of spheres $\mathbf{a} = \{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n\}$ lie in Q_0 , satisfy the non-overlapping restriction $\|\mathbf{a}_k - \mathbf{a}_j\| \geq 2r$ and the corresponding Delaunay graph Γ belong to a fixed class of graphs \mathcal{G} . Lemma 4.1 gives a bound for the packing problem in the fixed class \mathcal{G} . This bound yields the exact global minimum when the inequality (4.6) becomes an equality. Let some of the differences $|t_k - t_j|$ vanish and the rest of the differences $|t_k - t_j|$ are equal. If for the equal differences $|t_k - t_j|$, the differences $\|\mathbf{a}_k - \mathbf{a}_j\|$ are also equal we have got this exact global minimum. Actually, such a situation frequently met, for instance for graphs corresponding to laminated lattices.

Example 4.2. Consider the class of graphs \mathcal{A}_2 in \mathbb{R}^2 with $n = m^2$ ($m \in \mathbb{N}$) vertices containing the hexagonal lattice A_2 . This class is determined by the kissing number $N_k = 6$ for all the disks. The first step in the proof of optimality of the hexagonal lattice is the proof of equality $N_k = 6$. Here, we

refer to [11]. Hence, if we restrict ourselves by the class \mathcal{A}_2 , we do not go out a set of graphs containing the optimal packing.

The second step consists in the direct check that the regular hexagonal lattice satisfies (4.8). After, a simple external flux has to be applied and the corresponding $|t_k - t_j|$ and $\|\mathbf{a}_k - \mathbf{a}_j\|$ have to be calculated. Consider the regular hexagonal lattice generated by the vectors

$$\boldsymbol{\nu}_1 = (m, 0), \quad \boldsymbol{\nu}_2 = \left(m \cos \frac{\pi}{3}, m \sin \frac{\pi}{3}\right). \quad (4.15)$$

The radius of disks holds $r = \frac{1}{2}$. The periodicity cell Q_0 is determined by the vectors (4.15). It is convenient to consider A_2 as a laminated lattice with layers perpendicular to the axis x_2 . Introduce the number of the layer $q \in \mathbb{Z}$, where the q th layer consists of the disks whose centers have the x_2 -coordinate equal to $\frac{\sqrt{3}}{2}q$ (see Figure 3). Let the external flux be directed along the axis

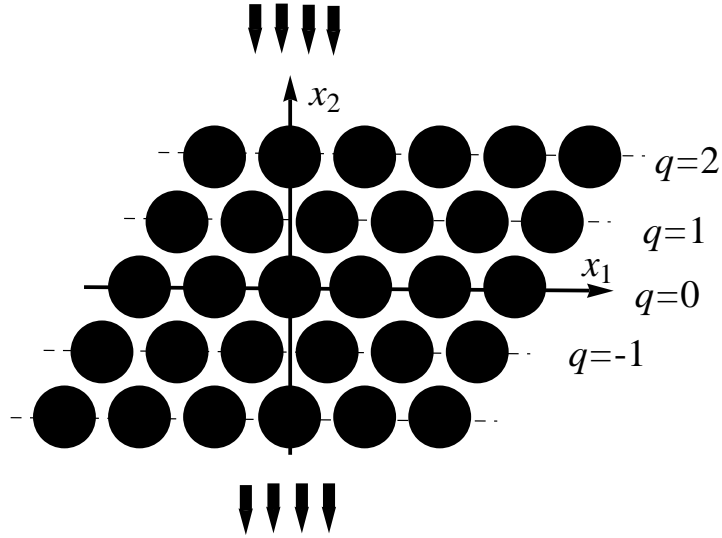


Figure 3: Hexagonal lattice as a laminated lattice with layers $q \in \mathbb{Z}$. The external flux is perpendicular to the axis x_1 .

x_2 and it is determined by the external potential $u_0(\mathbf{x}) = \frac{\sqrt{3}}{2}x_2$. Then the continuous and discrete potentials take the value q on all the disks of the q th layer. Therefore, the difference $|t_k - t_j|$ is equal to zero if \mathbf{a}_k and \mathbf{a}_j belong the same layer and it is equal to unity if \mathbf{a}_k and \mathbf{a}_j belong neighbor layers. The difference $\|\mathbf{a}_k - \mathbf{a}_j\|$ takes the same value $2r = 1$ for touching disks from neighbor layers. The inequality (4.6) becomes an equality in this case. It follows from Lemma 4.1 that the global minimum (4.1) on the class

of graphs \mathcal{A}_2 is attained at the regular hexagonal graph. The optimal location \mathbf{a}_* satisfies (4.8), hence depend on the basic vectors $\boldsymbol{\nu}_1$ and $\boldsymbol{\nu}_2$. If we take other basic vectors different from (4.15), we arrive at the optimal location \mathbf{a}_* which is not macroscopically isotropic.

This example gives an alternative "physical" proof of the optimal 2D packing attained for the hexagonal array but the first step of the proof contains equation $N_k = 6$ established by geometrical arguments.

Example 4.3. Consider the class of graphs \mathcal{Z}^2 in \mathbb{R}^2 with $n = m^2$ ($m \in \mathbb{N}$) vertices containing the square lattice \mathbb{Z}^2 . This class is determined by the contact number $N_k = 4$ for all the disks.

Consider the regular square lattice generated by the vectors $\boldsymbol{\nu}_1 = (m, 0)$ and $\boldsymbol{\nu}_2 = (0, m)$. The periodicity cell Q_0 is determined by these basic vectors. In accordance with the structural approximation theory the corresponding Delaunay graph³ consists of the edges parallel to the axes x_1 and x_2 . The lattice \mathbb{R}^2 is laminated with layers perpendicular to the axis x_1 . The q th layer consists of the disks whose centers have the x_2 -coordinate equal to q . The external flux is determined by the external potential $-u_0(\mathbf{x}) = -x_2$. Then the continuous and discrete potentials take the value q on all the disks of the q th layer. The further arguments repeat the previous example. Lemma 4.1 implies that the global minimum (4.1) on the class of graphs \mathcal{Z}^2 is attained at the regular square graph.

It is worth noting that the regular square lattice \mathbb{Z}^2 gives the optimal packing in the class \mathcal{Z}^2 . One can see that the class \mathcal{Z}^2 can be considered as unstable. It contains only one element \mathbb{Z}^2 , since any perturbation of a vertex yields flipping and changes the structure of \mathcal{Z}^2 .

Example 4.4. Consider the class of graphs \mathcal{A}_3 in \mathbb{R}^3 with $n = m^3$ ($m \in \mathbb{N}$) vertices containing the regular face-centered cubic lattice A_3 . Since this lattice has the laminated structure, we can consider the external flux directed perpendicular to the layers. Then, the potential is constant in each layer and the differences $\|\mathbf{a}_k - \mathbf{a}_j\| = 2r$ are constant where the neighbor points $\mathbf{a}_k, \mathbf{a}_j$ belong to the neighbor layers. This implies that the lattice A_3 reaches the optimal packing in the class \mathcal{A}_3 . It is worth noting that the optimal location \mathbf{a}_* in the class \mathcal{A}_3 depends on the basic vectors prescribed to the fcc lattice A_3 since \mathbf{a}_* satisfies the system (4.8) whose the right hand side depends on the basic vectors. The class of graphs containing the lattice corresponding to the hexagonal close-packing determines another optimal location, of course the hcp.

³It does not formally produce a Delaunay triangulation in the commonly used sense.

A class of graphs containing A_3 with arbitrary fixed basic vectors determines its optimal location \mathbf{a}_* through the system (4.8). This location \mathbf{a}_* depends on the basic vectors and must determine a macroscopically isotropic structure. The latter condition implies that the basic vectors have to correspond only to the fcc and hcp structures.

Perhaps, the kissing number $N_k = 12$ determines the class containing the optimal packing. This argument could give an alternative proof of the optimal packing for the regular fcc lattice [7].

These examples can be extended to the general space. Consider the class of graphs \mathcal{A}_d in \mathbb{R}^d containing a regular laminated lattice Λ_d . Then, the regular lattice Λ_d yields the optimal packing in the class \mathcal{A}_d .

5 Discussion

The most important fact used in this paper that the solution to the physical problem of the minimal energy (effective conductivity) implies solution to the geometrical problem of the optimal packing. Lemma 4.1 yields upper bounds for the classical optimal packing problem. For laminated structures these bounds are exact, hence solve the optimal packing problems within the considered classes. Lemma 4.1 yields not only upper bounds but an effective algorithm for their computations, since the linear system (4.8) is decomposed onto d independent systems with n equations.

Therefore, we solve the optimal packing problem in any fixed class of graphs \mathcal{G} . Let us discuss these classes of graphs. Though the number of spheres per cell n is arbitrary and can tend to infinity, the periodicity cell is fixed at the beginning, hence the optimal location \mathbf{a}_* depends on the basic vectors. It follows also from the observation that the right hand part of the system (4.8) contains the basic vectors. For sufficiently large n , the majority of equations of (4.8) are homogeneous and only "boundary" equations are inhomogeneous. Their number is of order \sqrt{n} . It is interesting to investigate the asymptotic dependence of \mathbf{a}_* on the basic elements as $n \rightarrow \infty$. This will show, for instance, the effectiveness of the hexagonal type packing in the cubic cell in \mathbb{R}^d .

We do not know a priori from the cell Q_0 and structure of \mathcal{G} that the solution \mathbf{a}_* of the system (4.8) will form a macroscopically isotropic structure. However, a simple necessary condition of isotropy can be checked: the location \mathbf{a}_* must contain d percolation chains connecting the opposite face of the parallelotope Q_0 (see Fig.2).

A straight forward verification which class \mathcal{G} yields optimal packing can be proposed for a fixed n . First, for clarity consider 1D case. Then there

exists exactly one class of graph \mathcal{Z} including the regular 1D lattice \mathbb{Z} . A graph from \mathcal{Z} consists of sequentially located edges along the axis. It follows from the system (4.8) that each point a_k lies in the middle of the segment (a_{k-1}, a_{k+1}) that immediately implies the points a_k form the lattice \mathbb{Z} . The following extension of the above scheme to \mathbb{R}^d can be proposed. Let $x_p^{(k)}$ denote the p th coordinate of the point \mathbf{a}_k ($p = 1, 2, \dots, d$). All the points $x_p^{(k)}$ ($k = 1, 2, \dots, n$) are located on the real axis \mathbb{R} (coincidence is permitted) and satisfy the system

$$x_p^{(k)} = \frac{1}{N_k} \sum_{j \in J_k} x_p^{(j)} + \frac{1}{N_k} \sum_{\ell=1}^d s_{j\ell} \nu_p^{(\ell)}, \quad k = 1, 2, \dots, n, \quad (5.1)$$

where $\nu_p^{(\ell)}$ denotes the p th coordinate of the basic vector $\boldsymbol{\nu}_\ell$. The class of graphs \mathcal{G} determines the sets J_k , i.e., connections between the points $x_p^{(k)}$ and $s_{j\ell}$. In particular, \mathcal{G} determines N_k restricted by the kissing number. It is important to solve the system (5.1) keeping the parameters $\nu_p^{(\ell)}$ in symbolic form. It can be done by separate numerical solutions to the systems

$$x_p^{(k\ell)} = \frac{1}{N_k} \sum_{j \in J_k} x_p^{(j\ell)} + \frac{s_{j\ell}}{N_k}, \quad k = 1, 2, \dots, n, \quad (5.2)$$

and by the linear combination

$$x_p^{(k)} = \sum_{\ell=1}^d x_p^{(k\ell)} \nu_p^{(\ell)}, \quad k = 1, 2, \dots, n. \quad (5.3)$$

All the computations can be made separately for $p = 1, 2, \dots, d$. As a result we obtain expressions for the optimal \mathbf{a}_k in the class \mathcal{G}

$$\mathbf{a}_k = \sum_{\ell=1}^d \mathbf{a}_k^{(\ell)} \boldsymbol{\nu}_\ell, \quad k = 1, 2, \dots, n, \quad (5.4)$$

where the vectors $\mathbf{a}_k^{(\ell)}$ are given numerically. The next numerical problem consists in determinations of such bases $\{\boldsymbol{\nu}_\ell\}_{\ell=1}^d$ which possess d percolation chains connecting the opposite faces of the parallelotope Q_0 . Ultimately, one has to perform this procedure for all the classes of graphs and take the best packing. The above algorithm is rather an idea how to apply solution to the packing problem within classes \mathcal{G} to the traditional sphere packing [5], [7].

The physical problem is considered in the class of periodic structures. General non-periodic composites were discussed in literature (see a review

in [8] and references therein). The main question consists in extension of the structural approximation theory [2], [8] developed for densely packed composites to the non-periodic case.

We do not discuss the case of different radii. We suppose that a similar work can be done, since simple formulae for $g_{jk}^{(0)}$ are known [2], [8] and can be extended to \mathbb{R}^d following Sec.3.

References

- [1] Bakhvalov, N.S., Panasenko, G.P.: Homogenization: Averaging processes in periodic media. Nauka, Moscow (1984) [in Russian]; English transl. Kluwer, Dordrecht /Boston /London (1989)
- [2] Berlyand, L., Kolpakov, A.G., Novikov, A.: Introduction to the Network Approximation. Method for Materials Modeling. Cambridge University Press, Cambridge (2013)
- [3] Bezdek, K.: Lectures on Sphere Arrangements - the Discrete Geometric Side. Springer, New York etc (2013).
- [4] Bezdek, K., Deza, A., Ye, Yinyu (Eds.): Discrete Geometry and Optimization. Springer, New York etc (2013).
- [5] Conway, J., Sloane, N.J.A.: Sphere Packings, Lattices and Groups. Springer, New York etc (1999)
- [6] Keller, J.B.: Conductivity of a Medium Containing a Dense Array of Perfectly Conducting Spheres or Cylinders or Nonconducting Cylinders. J. Appl. Phys. 34, 991-993 (1963)
- [7] Lagarias, J.C. (Ed.): The Kepler Conjecture: The Hales-Ferguson Proof. Springer, New York etc (2011)
- [8] Kolpakov, A.A., Kolpakov, A.G.: Capacity and Transport in Contrast Composite Structures: Asymptotic Analysis and Applications. CRC Press, Boca Raton (2010)
- [9] Mityushev V., Rylko N.: Optimal distribution of the non-overlapping conducting disks. Multiscale Model. Simul. 10, 180-190 (2012)
- [10] Rylko N.: Structure of the scalar field around unidirectional circular cylinders. Proc. R. Soc. A464, 391-407 (2008)

- [11] Tóth, L. Fejes: Lagerungen in der Ebene auf der Kugel und im Raum.
Springer-Verlag, Berlin, New York (1953)